

## Step-by-step simulation of radiation chemistry using Green functions for diffusion-influenced reactions

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Radiolytic species are formed  $\sim 1$  ps after the passage of ionizing radiation through matter. After their formation, they diffuse and chemically react with other radiolytic species and neighboring biological molecules, leading to various oxidative damage. Therefore, the simulation of radiation chemistry is of considerable importance to understand how radiolytic species damage biological molecules [1]. The step-by-step simulation of chemical reactions is difficult, because the radiolytic species are distributed non-homogeneously in the medium. Consequently, computational approaches based on Green functions for diffusion-influenced reactions should be used [2]. Recently, Green functions for more complex type of reactions have been published [3-4]. We have developed exact random variate generators of these Green functions [5], which will allow us to use them in radiation chemistry codes. Moreover, simulating chemistry using the Green functions is which is computationally very demanding, because the probabilities of reactions between each pair of particles should be evaluated at each timestep [2]. This kind of problem is well adapted for General Purpose Graphic Processing Units (GPGPU), which can handle a large number of similar calculations simultaneously. These new developments will allow us to include more complex reactions in chemistry codes, and to improve the calculation time. This code should be of importance to link radiation track structure simulations and DNA damage models.

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